

Butanoic anhydride
106-31-0 | DTXSID8026729

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: $5.09\text{e-}12\text{ cm}^3/\text{molecule}\cdot\text{sec}$

Global applicability domain: Inside

Local applicability domain index: $5.02\text{e-}01$

Confidence level: $7.51\text{e-}01$

Nearest Neighbors from the Training Set

[Image not found](#)

Dimethyl adipate

Measured: $8.40\text{e-}12$

Predicted: $6.84\text{e-}12$

[Image not found](#)

Dimethyl glutarate

Measured: $3.30\text{e-}12$

Predicted: $3.76\text{e-}12$

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Dimethyl succinate

Measured: $1.40\text{e-}12$

Predicted: $1.93\text{e-}12$

[Image not found](#)

2-Ethoxyethyl isobutyrate

Measured: $1.35\text{e-}11$

Predicted: $1.28\text{e-}11$

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Ethyl 3-ethoxypropionate

Measured: $2.29\text{e-}11$

Predicted: $1.63\text{e-}11$